

ABSTRACT

METHOD FOR GENERATING A DATABASE OF MOLECULAR FRAGMENTS

- 5       A method is provided of generating a database of molecular fragment data defining parts of molecular structures, from a data set containing data describing predetermined molecular structures. The method comprises:-
- 10      a) selecting first and second molecular structure data defining first and second molecular structures respectively from the data set;
- 10      b) comparing the selected data to determine molecular fragment data which defines at least part of a molecular structure common to each of the first and second molecular structures;
- 15      c) storing the determined molecular fragment data in the data set; and,
- 15      d) repeatedly performing steps (a) to (c) wherein either of the first or the second molecular structure data is selected from either the predetermined molecular structure data or the molecular fragment data determined in step (b) such that the resultant data set comprises a database containing the molecular fragment data.